



Trading Performance for Memory in Sparse Direct Solvers using Low-rank Compression

Loris Marchal, Thibault Marette, Grégoire Pichon, Frédéric Vivien

► To cite this version:

Loris Marchal, Thibault Marette, Grégoire Pichon, Frédéric Vivien. Trading Performance for Memory in Sparse Direct Solvers using Low-rank Compression. [Research Report] RR-9368, INRIA. 2020. hal-02976233

HAL Id: hal-02976233

<https://inria.hal.science/hal-02976233>

Submitted on 23 Oct 2020

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.



Trading Performance for Memory in Sparse Direct Solvers using Low-rank Compression

Loris Marchal, Thibault Marette, Grégoire Pichon, Frédéric Vivien

**RESEARCH
REPORT**

N° 9368

October 2020

Project-Team ROMA

ISRN INRIA/RR--9368--FR+ENG

ISSN 0249-6399



Trading Performance for Memory in Sparse Direct Solvers using Low-rank Compression

Loris Marchal*, Thibault Marette*, Grégoire Pichon*, Frédéric Vivien*

Project-Team ROMA

Research Report n° 9368 — October 2020 — 28 pages

Abstract: Sparse direct solvers using Block Low-Rank compression have been proven efficient to solve problems arising in many real-life applications. Improving those solvers is crucial for being able to 1) solve larger problems and 2) speed up computations. A main characteristic of a sparse direct solver using low-rank compression is *when* compression is performed. There are two distinct approaches: (1) all blocks are compressed before starting the factorization, which reduces the memory as much as possible, or (2) each block is compressed as late as possible, which usually leads to better speedup. The objective of this paper is to design a composite approach, to speedup computations while staying under a given memory limit. This should allow to solve large problems that cannot be solved with Approach 2 while reducing the execution time compared to Approach 1. We propose a *memory-aware* strategy where each block can be compressed either at the beginning or as late as possible. We first consider the problem of choosing when to compress each block, under the assumption that all information on blocks is perfectly known, i.e., memory requirement and execution time of a block when compressed or not. We show that this problem is a variant of the NP-complete Knapsack problem, and adapt an existing 2-approximation algorithm for our problem. Unfortunately, the required information on blocks depends on numerical properties and in practice cannot be known in advance. We thus introduce models to estimate those values. Experiments on the PASTIX solver demonstrate that our new approach can achieve an excellent trade-off between memory consumption and computational cost. For instance on matrix Geo1438, Approach 2 uses three times as much memory as Approach 1 while being three times faster. Our new approach leads to an execution time only 30% larger than Approach 2 when given a memory 30% larger than the one needed by Approach 1.

Key-words: Sparse direct solvers, Low-rank compression, Scheduling, Memory constraints

* Univ Lyon, EnsL, UCBL, CNRS, Inria, LIP, F-69342, LYON Cedex 07, France

RESEARCH CENTRE
GRENOBLE – RHÔNE-ALPES

Inovallée
655 avenue de l'Europe Montbonnot
38334 Saint Ismier Cedex

Compromis temps/mémoire pour les solveurs directs creux utilisant de la compression low-rank

Résumé : Les solveurs directs creux utilisant de la compression low-rank ont montré leur efficacité pour résoudre de grands systèmes. Les améliorer permet de 1) résoudre de plus grands problèmes et 2) accélérer la résolution. Une caractéristique principale de ces solveurs est *quand* la compression est réalisée. Il existe deux approches: (1) tous les blocs sont compressés avant le début de la factorisation, ce qui minimise la consommation mémoire, ou (2) chaque bloc est compressé au plus tard, ce qui permet d'avoir de meilleures performances. L'objectif de cet article est de proposer une approche intermédiaire, qui accélère les calculs au maximum tout en restant en dessous d'une limite mémoire donnée. Cela devrait permettre de résoudre de grands problèmes que l'approche 2 ne peut pas résoudre ou de réduire le temps d'exécution de l'approche 1. Nous proposons une stratégie *memory-aware* où chaque bloc peut être compressé au début ou au plus tard. Nous commençons par considérer le problème où toutes les informations (consommation mémoire et temps d'exécution en version compressée ou non) sont parfaitement connues. Nous montrons que ce problème est une variante du problème NP-complet Knapsack et adaptons une 2-approximation pour notre problème. Malheureusement, toutes ces informations dépendent de propriétés numériques et ne sont pas connues à l'avance. Des modèles sont donc introduits afin d'estimer ces valeurs. Des expérimentations avec le solveur PASTIX montrent que notre approche permet d'avoir un excellent compromis entre consommation mémoire et temps d'exécution. Par exemple, pour la matrice Geo1438, l'approche 2 utilise trois fois plus de mémoire que l'approche 1, qui est trois fois plus lente. Notre nouvelle méthode permet d'obtenir à la fois un temps d'exécution seulement 30% supérieur à celui de l'approche 2 tout en ayant une consommation mémoire seulement supérieure de 30% à celle de l'approche 1.

Mots-clés : Solveurs directs creux, Compression Low-rank, Ordonnancement, Contraintes mémoire

1 Introduction

Many numerical applications such as computational fluid dynamics, electromagnetism, or structural mechanics use numerical models that require solving systems of the form $Ax = b$, where A is a sparse matrix of size n , meaning that the number of non-zero elements is in $\Theta(n)$. Sparse matrices appear for instance when discretizing Partial Differential Equations (PDEs) on 2D and 3D finite element or finite volume meshes: each point interacts only with its neighborhood. Solving large sparse linear systems is an expensive operation, thus enhancing this step is of interest for many real-life applications. Among the methods available to solve sparse linear systems, sparse direct solvers are widely used for their numerical robustness that allows to tackle most problems. However, both the memory footprint and the number of operations limit the use of sparse direct solvers for very large matrices. To circumvent this problem, a recent approach consists of compressing some blocks appearing during the factorization with low-rank compression techniques. The objective is then to reduce the computational cost and the memory footprint while losing some numerical information in a controlled way. As many applications do not require to get a solution at the machine precision, this approach is now used in various contexts. Low-rank compression can thus appear as a perfect solution because it may both decrease computational cost and memory footprint. While this is true on parts of the computations (computing the updates), using low-rank compression can also increase the computational costs on other parts of the computations (applying the updates). In particular, when used to drastically reduce the memory footprint, low-rank compression usually ends up increasing the total processing time compared to versions that use temporary memory spaces.

There exist different formats to represent a matrix into a compressed form. Among them, Block Low-Rank (BLR) compression consists of splitting a matrix into regular blocks before compressing independently each block, for instance with Singular Value Decomposition (SVD). This approach has been used for the MUMPS [1,2] and the PASTIX [3] sparse direct solvers and has been proven efficient for many real-life problems. The other type of representation relies on a recursive splitting of the matrix and has led to several formats: \mathcal{H} [4], \mathcal{H}^2 [5], HSS [6], and HODLR [7] for instance. The approach commonly used in those solvers is to compress large dense blocks appearing during the factorization of a sparse matrix and not the sparse matrix itself. In this paper, we will focus on the BLR format.

If sparse direct solvers using BLR compression have demonstrated good results, allowing to solve large problems and/or to significantly reduce the time-to-solution, there are still limitations that prevent solving large systems with a huge level of parallelism when working under some memory constraints. In the MUMPS solver, some large blocks, namely the fronts, are fully allocated (in dense format) before being compressed during the factorization. Thus, this reduces the potential memory gain as those blocks exist in their full-rank form before being compressed. In the PASTIX solver, two approaches have been developed,

a first one significantly reducing execution time without carefully managing the memory consumption and a second one much slower that minimizes as much as possible the memory footprint.

The objective of this paper is to propose a new memory-aware strategy for the PASTIX solver that does not minimize the memory consumption but keeps it under a given memory limit, utilizing as much as possible the available resources. The idea is to perform as many computationally efficient but memory expensive operations as possible while allowing some time overhead for some computationally expensive but memory thrifty operations if the memory used would exceed the memory available on the machine.

The main contributions of this paper are the following:

- We propose a *memory-aware* strategy that allows each block to be compressed either as early as possible, or as late as possible, independently from the choice of other blocks.
- We show that the offline problem (with perfect information available) of choosing which blocks to compress at the beginning is a variant of the Knapsack problem, and that all approximation algorithms for Knapsack can be adapted as approximation algorithms for our problem with the same ratio.
- We design models to estimate the information needed by these approximation algorithms, namely the size of the compressed blocks and their update times in the compressed and non-compressed formats.
- We provide a proof-of-concept implementation of a dynamic version of the proposed *memory-aware* strategy in the PASTIX solver. Our results on actual matrices demonstrate the large potential of the proposed approach, leading to excellent trade-offs between memory and performance.

We stress that the proof-of-concept implementation of the proposed strategy uses the sequential version of the PASTIX solver, even if the parallel version is clearly our final objective. There are two reasons for this limitation: (i) adapting the dynamic strategy to a parallel and distributed solver such as PASTIX would require non-trivial work to resolve synchronization problems, and (ii) the work presented here is needed to first assess the interest of our approach. Therefore, the present study is a necessary building block.

The rest of the paper is organized as follows. In Section 2, we present some background on sparse linear solvers and low-rank compression before detailing the problem studied and the objectives of the paper. In Section 3, we formalize the problem and prove that it is NP-hard before presenting a low complexity approximation algorithm. In Section 4, we present models to evaluate the cost and the memory footprint associated to each block. Combining the formalization of the problem and the predictive models, we present the results of the new strategy for the PASTIX solver in Section 5, before concluding this work in Section 6.

2 Background and Proposed Approach

Introducing low-rank compression in sparse direct solvers brings the problem of *when* to perform the compression of data blocks. In Section 2.1 we briefly present the different steps of sparse direct solvers. In Section 2.2, we describe how low-rank compression can be used to reduce the memory consumption and/or the time-to-solution. In Section 2.3, we present the idea driving this paper, that is, to reduce as much as possible time-to-solution while satisfying a memory constraint. In Section 2.4, we comment the position of the literature with respect to this open problem.

2.1 Sparse direct solvers

This section intends to briefly present sparse direct solvers. For more details, see [8] for instance. In order to solve $Ax = b$, a sparse direct solver factorizes the matrix A into a product of triangular matrices, following the Gauss elimination. In the general case, when the matrix is not symmetric, one can compute $A = LU$, where L is a lower triangular matrix and U an upper triangular matrix. Then the system can be solved by performing triangular solves: we solve $Ly = b$ and then $Ux = y$.

Solving a sparse system with a sparse direct solver is usually divided into four main steps: 1) Ordering the unknowns to minimize the fill-in, i.e., null elements becoming non-zeroes during the factorization; 2) Computing the block symbolic factorization, that predicts the form of the factorized matrix before any numerical operations take place; 3) Factorizing the matrix; 4) Solving triangular systems.

The first step, ordering the unknowns, is usually performed using the nested dissection algorithm [9] through external partitioning tools such as METIS [10] or SCOTCH [11]. From this process, unknowns are grouped together into sets that will correspond to column blocks in the following block symbolic factorization.

The second step, building the block symbolic factorization, intends to represent the sparse matrix as a collection of dense blocks. A sparse matrix can be seen as a set of column blocks, each corresponding to a set of unknowns issued from the nested dissection. It is composed of a dense diagonal block, representing the interactions between the unknowns of the column block, and several off-diagonal blocks (located either below on the same columns or on the right on the same rows as the diagonal block), that represent the interactions with other column blocks. Figure 1 presents such a structure for a small matrix. In order to increase the level of parallelism, large diagonal blocks (and thus large column blocks) can be split into smaller blocks, increasing the overall number of column blocks. The objective of this block structure is to split the data among blocks that remain large enough to leverage efficient BLAS level 3 [12] operations.

Once this step is performed, all the blocks (either diagonal or off-diagonal) can be initialized with the original values of A , before performing the numerical factorization. The latter follows the Gauss elimination as for dense matrices, but the sparsity is carefully managed to operate only on blocks not entirely

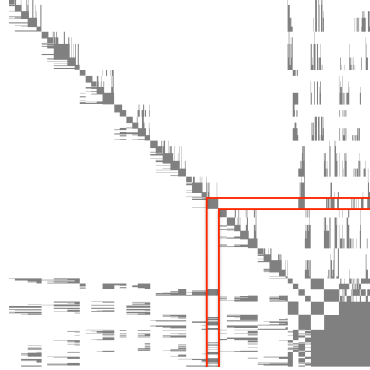


Figure 1: Symbolic factorization of a $10 \times 10 \times 10$ Laplacian. The red lines define the blocks grouped into a single column block: one diagonal block and several off-diagonal blocks.

made of zeroes. The following operations take place to treat (or eliminate) each column block, one after the other: 1) **Factorize** the dense diagonal block, 2) Eliminate (**Solve**) off-diagonal blocks belonging to that column block and 3) **Update** that performs a matrix-matrix product between each couple of off-diagonal blocks belonging to the column block before applying the contribution to the trailing sub-matrix. This step will be detailed in Section 2.2.

Finally, the triangular solves can be performed once the matrix is factorized.

2.2 Low-rank compression

Although sparse direct solvers are well-known for their numerical stability, their main limitation is their complexity, both for memory storage and number of operations. The storage corresponds to each gray block on Figure 1, while the time complexity mostly comes from the **Update** process, where a matrix-matrix product is performed between each couple of off-diagonal blocks belonging to the column block.

The BLR compression consists of compressing large off-diagonal blocks. Note that when compressing a block A of size $m \times n$, we obtain a low-rank form $u_A v_A^t$, where u_A is of size $m \times r_A$ and v_A of size $n \times r_A$, r_A being the rank of the matrix A . Diagonal blocks remain dense. Remember that large diagonal blocks have been split among smaller blocks during the block symbolic factorization. Thus, from the refined symbolic factorization, only small diagonal blocks remain. Depending on *when* the low-rank compression is performed, the numerical factorization process is modified accordingly. We will now present two strategies introduced into the PASTIX [13] solver, presented in [3].

2.2.1 Minimal Memory – low-rank updates

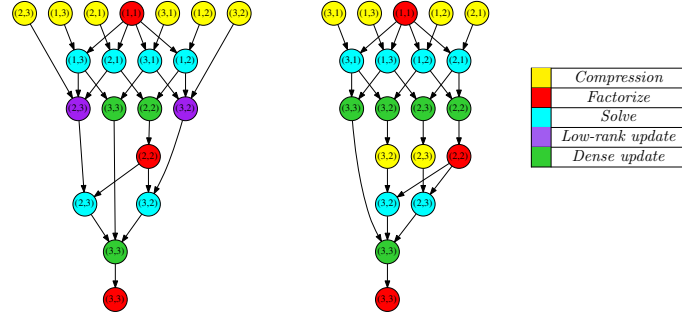
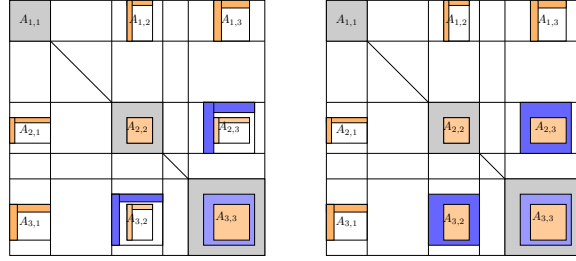
A first strategy, namely *Minimal Memory*, consists of compressing all large off-diagonal blocks before starting the numerical factorization. The main asset of this approach is that blocks are never allocated in their full-rank form, thus dramatically reducing the memory footprint of the solver. However, it raises the problem of updating low-rank blocks.

On Figure 2(b), we present a partial sparse matrix at the step of eliminating column block 1. (An uncompressed matrix is represented by a full rectangle, like block $A_{(2,2)}$ and a compressed matrix by two small rectangles, like block $A_{(2,1)}$.) The corresponding Direct Acyclic Graph (DAG) of tasks is presented on left of Figure 2(a). The matrix on Figure 2(b) corresponds to the tasks shown on the third row of the DAG. In this strategy, blocks are compressed at the beginning of the factorization with the *Compression* kernel. Thus, instead of performing only full-rank updates, some low-rank matrices are updated with the *Low-rank update* kernel. For instance, block $A_{(3,2)}$ receives a contribution made of the product of blocks $A_{(3,1)}$ and $A_{(1,2)}$, corresponding to a *Low-rank update* task on the DAG on Figure 2(a). This operation is split into two parts: producing a low-rank contribution $u_{AB}v_{AB}^t = (u_{A_{(3,2)}} v_{A_{(3,2)}}^t)(u_{A_{(3,1)}} v_{A_{(3,1)}}^t)$ (see [3] for detail) and applying this contribution $A_{(3,2)} - = u_{AB}v_{AB}^t$. As depicted on Figure 2(d), updating a low-rank block with several low-rank contributions consists of utilizing dedicated kernels to maintain a low-rank structure. Producing the contribution $u_{AB}v_{AB}^t$ is faster than in the full-rank case, while applying this contribution can be expensive.

One can see that due to sparse properties, the target (that is, the block to be updated) may be much larger than some contributing blocks (for example, $contrib_2$ is much smaller than C_1 in Figure 2(d)). This is the drawback of this approach, as the complexity of updating a low-rank target depends on its size and not on the size of the smaller contribution. Note that the rank of the target block can grow with the updates, thus the size of the low-rank structure slowly increases before reaching its final size when receiving the last contribution. The rank may also decrease due to particular numerical properties (updates that cancel previous contributions), but this behavior is rarely observed in practice.

2.2.2 Just-In-Time – full-rank updates

Another strategy introduced in the PASTIX solver consists of compressing blocks as late as possible, once they have received all their contributions and thus will not be updated anymore. This strategy is named *Just-In-Time*. Figure 2(c) presents the partial matrix obtained when eliminating the column block 1. One can see that off-diagonal blocks belonging to column block 2 are not compressed yet. The right part of Figure 2(a) presents the DAG of the corresponding operations. As the target blocks are now full-rank, the cost of applying the updates is as cheap as for the full-rank version of the solver. Thus, similarly to the *Minimal Memory* strategy, the cost is reduced when computing matrix-matrix products between low-rank matrices, while there is no extra overhead

(a) DAGs: *Minimal Memory* on left, *Just-In-Time* on right.(b) Eliminating column block 1 with *Minimal Memory* strategy.(c) Eliminating column block 1 with *Just-In-Time* strategy.

$$\begin{aligned}
 C_1 &= \text{Low-rank update} \left(\begin{array}{c} \text{gray bar} \\ \text{gray bar} \end{array}, \begin{array}{c} \text{blue bar} \\ \text{blue bar} \end{array} \right) \\
 C_{\text{final}} = C_2 &= \text{Low-rank update} \left(\begin{array}{c} \text{gray bar} \\ \text{gray bar} \end{array}, \begin{array}{c} \text{green bar} \\ \text{green bar} \end{array} \right)
 \end{aligned}$$

(d) Updates with *Minimal Memory* strategy.

$$\begin{aligned}
 C_1 &= \text{Dense update} \left(\begin{array}{c} \text{gray bar} \\ \text{gray bar} \end{array}, \begin{array}{c} \text{blue bar} \\ \text{blue bar} \end{array} \right) \\
 C_{\text{final}} &= \text{Compression} \left(\begin{array}{c} \text{gray bar} \\ \text{gray bar} \end{array} \right) = \text{Dense update} \left(\begin{array}{c} \text{gray bar} \\ \text{gray bar} \end{array}, \begin{array}{c} \text{green bar} \\ \text{green bar} \end{array} \right)
 \end{aligned}$$

(e) Updates with *Just-In-Time* strategy.Figure 2: DAGs, state of the matrix when elimination column block 1 and example of updating a block with two contributions for *Minimal Memory* and *Just-In-Time* strategies.

when updating the target matrix.

In the DAG of tasks, instead of compressing all large off-diagonal blocks before the beginning of the factorization, those blocks are compressed throughout the computation, as depicted with the *Compression* kernel that appears on lines 1 and 4 of the DAG. The *Low-rank update* kernel that appeared for the *Minimal Memory* strategy is not used anymore. As presented on Figure 2(e), an update consists now of forming the dense contribution and applying it directly to the target matrix. For instance, block $A_{(3,2)}$ receives a contribution made of the product of blocks $A_{(3,1)}$ and $A_{(1,2)}$. This product can be represented as a low-rank matrix $u_{AB}v_{AB}^t$, as in Section 2.2.1. The full-rank contribution is explicitly built before being applied to $A_{(3,2)}$. There is a huge gain when computing the matrix-matrix product between low-rank matrices, while there is no extra overhead when applying this product.

2.3 Towards a new mixed strategy

The *Minimal Memory* strategy was introduced to consume as little memory as possible, while the *Just-In-Time* strategy is dedicated to reduce time-to-solution. If the matrix fits in memory, it is thus more interesting to use the *Just-In-Time* strategy, while it has been shown in [3] that the *Minimal Memory* strategy allows to solve problems that are too large to be solved with either the full-rank or the *Just-In-Time* strategy. An intermediate approach which would better meet the needs of real-life users would be to use as much as possible the *Just-In-Time* strategy while moving to the *Minimal Memory* strategy if the memory consumption is too high.

In practice, let us consider the block $A_{(3,2)}$ that appears on both Figure 2(b) and Figure 2(c). As presented on Figure 2(d) and Figure 2(e), the same contributions are applied on this block for both *Minimal Memory* and *Just-In-Time* strategies. In addition, after the block has received all its contributions, it is in a low-rank form (either it remains in that form, or it is compressed to reach it). Thus, the block **receives** and **produces** exactly the same information, no matter if the *Minimal Memory* or the *Just-In-Time* strategy was used. Then it is possible, for a same factorization, to compute a subset of blocks using the *Minimal Memory* strategy and the remaining blocks with the *Just-In-Time* strategy. It is even possible to compress a block in “the middle” of the factorization, *i.e.*, applying first full-rank updates and then low-rank updates.

For instance, instead of using either the *Just-In-Time* strategy (as depicted on Figure 2(c)) or the *Minimal Memory* strategy (as depicted on Figure 2(b)), one could imagine to have $A_{(3,2)}$ compressed **early** before the beginning of the factorization and $A_{(2,3)}$ compressed in a **lazy** way as it happens with the *Just-In-Time* strategy.

The objective of this paper is to propose an intermediate strategy that chooses which blocks to execute following the *Just-In-Time* strategy and which ones to execute following the *Minimal Memory* strategy in order to respect a given memory constraint. Thus, the approach we study in this paper combines the assets of both existing strategies: allowing to solve very large problems while

utilizing as many efficient operations as possible.

2.4 Related work

Up to our knowledge, this work is the first tentative to combine both low-rank and full-rank updates in a sparse solver. Most solvers using low-rank compression are performing full-rank updates, which favor the reduction of execution time.

There are few works that propose an implementation of a low-rank solver using low-rank updates. In [14], such an approach is proposed, but the performance obtained is low, slower than a generic sparse direct solver. The work conducted for the PASTIX solver [3], in a supernodal context, manages low-rank updates between blocks of different sizes. The widely used sparse direct solver MUMPS [1,2] relies on the multifrontal factorization. In this solver, a block is not allocated before the start of the factorization but only when it is needed. Some large blocks, however, the fronts, are fully allocated in their full-rank form after they have received all their contributions and before being compressed. In order to reduce this memory cost, either the allocation could be performed panel by panel or low-rank updates should be used. Thus, this work is of interest to the community as it provides an intermediate approach, using as much as possible efficient dense updates and moving to low-rank updates when necessary to stay under a given memory limit.

On a more general view, this study focuses on deriving space-time trade-offs using low-rank compression and scheduling. We refer the reader interested by general space-time trade-offs to [15, Chapter 10] or by memory-aware scheduling, in particular for DAGs, to [16].

3 Modelization of the problem

We now formalize the problem and describe how to decide which tasks should be computed with the *Minimal Memory* strategy and which ones should be performed with the *Just-In-Time* strategy. For the remaining of the paper, blocks following the *Minimal Memory* strategy will be said to be in *early* mode, while blocks following the *Just-In-Time* strategy will be said to be in *lazy* mode.

In Section 3.1, we present the formalization of the problem. In Section 3.2, we demonstrate that this problem is equivalent to *Knapsack* and explicit the approximation algorithm that will be used in the remaining of the paper.

3.1 Formalization: *Makespan With Bounded Memory*

The objective here is to exhibit, among the off-diagonal blocks that are large enough to be compressed, two set of blocks, a first one to be performed in *early* mode and a second one to be performed in *lazy* mode, such that the total memory consumption of those blocks does not exceed a given bound.

We consider a set \mathcal{J} of n independent tasks, J_1, \dots, J_n , where a task J_i represents an off-diagonal block. Each task has an execution time, corresponding to the sum of all elementary updates (as presented on Figure 2(d) and Figure 2(e)) that are applied to the block and a memory consumption, which is the memory storage of the block. Both this time and this memory depend on the mode chosen for this block:

- If executed in the *lazy* mode (as in the *Just-In-Time* strategy), its execution takes a time t_i and uses a memory (storage) S_i ;
- Otherwise, in the *early* mode (as in the *Minimal Memory* strategy), its execution takes a time T_i and uses a memory (storage) s_i .

We make the assumption that executing a task in *lazy* mode takes less time and more memory than executing it in *early* mode. Therefore for any $i \in [1; n]$, $S_i > s_i$ and $T_i > t_i$. Otherwise, if $S_i \leq s_i$ it is always better to execute the task in *lazy* mode and if $T_i \leq t_i$ it is always better to use *early* mode.

mode / strategy	<i>lazy</i> / <i>Just-In-Time</i>	<i>early</i> / <i>Minimal Memory</i>
memory size	S_i	s_i
processing time	t_i	T_i

Table 1: Summary of key parameters.

All tasks are executed one after the other on a single processor; hence, the total processing time is the sum of all task execution times. In this model, we suppose that all tasks are simultaneously present in memory, from the beginning of the execution of the first task until the completion of the very last task. Let \mathcal{M} be the memory threshold, such that $\mathcal{M} \geq \sum s_i$, meaning that all tasks fit in memory if executed with the *early* mode. Note that we suppose here that the ranks of blocks are kept invariant during the factorization, while it is not exactly the case as presented in Section 2.2.

Definition 1 *The MakespanWithBoundedMemory problem consists of choosing for each task if it will be executed in early or in lazy mode, while respecting the memory constraint and minimizing the total processing time.*

3.2 Equivalence to *Knapsack* and heuristic to solve the problem

The *MakespanWithBoundedMemory* problem is actually exactly the *Knapsack* [17] problem.

Definition 2 *Knapsack problem: Let \mathcal{I} be a set of n items. Each item has a value v_i and a weight w_i . The objective is to fit some of the items in a bag of weight capacity W , while maximizing the value of the objects inside the bag.*

Theorem 1 *Knapsack and MakespanWithBoundedMemory are equivalent: any algorithm solving one problem can be used to solve the other.*

The intuition of this equivalence is the following. Consider that all tasks of *MakespanWithBoundedMemory* are initially in *early* mode, and we want to choose which ones to move to *lazy* mode. Chosen tasks will corresponds to chosen items in *Knapsack*. We first want the memory consumption to stay below the threshold \mathcal{M} . For each task moved to *lazy* mode, we pay an extra memory of $S_i - s_i$ compared to the original storage cost ($\sum s_i$). This corresponds to the knapsack constraint with weights $w_i = S_i - s_i$ and capacity $\mathcal{W} = \mathcal{M} - \sum s_i$. The objective is to minimize the execution time, and for each task moved to *lazy* mode, we earn a time $T_i - t_i$ compared to the initial time ($\sum T_i$). This corresponds to maximizing the sum of the values $v_i = T_i - t_i$ of the chosen items.

Proof 1 *Let us express MakespanWithBoundedMemory as an Integer Linear Problem (ILP):*

We associate a variable $x_i \in \{0, 1\}$ to each $J_i \in [1, n]$.

Let

- $x_i = 1$ if the task J_i is executed in *lazy* mode,
- $x_i = 0$ if the task J_i is executed in *early* mode.

Therefore, the ILP problem is:

$$\text{minimize} \quad \sum_{i=1}^n (x_i t_i) + \sum_{i=1}^n ((1 - x_i) T_i) \quad (1)$$

$$\text{subject to} \quad \sum_{i=1}^n (x_i S_i) + \sum_{i=1}^n ((1 - x_i) s_i) \leq \mathcal{M} \quad (2)$$

$$\text{and} \quad \forall i \in \{1, n\}, x_i \in \{0, 1\} \quad (3)$$

Moreover we have the following equivalence:

$$(1) \iff \text{maximize} \sum_{i=1}^n x_i (T_i - t_i) - \sum_{i=1}^n T_i$$

$$\iff \text{maximize} \sum_{i=1}^n x_i (T_i - t_i)$$

$$(2) \iff \sum_{i=1}^n x_i (S_i - s_i) \leq \mathcal{M} - \sum_{i=1}^n s_i$$

Thanks to this two equivalences, we just showed that the ILP is exactly a linear formulation of the Knapsack problem:

$$\text{maximize} \quad \sum_{i=1}^n x_i v_i$$

$$\text{subject to} \quad \sum_{i=1}^n x_i w_i \leq \mathcal{W}$$

$$\text{and} \quad \forall i \in \{1, n\}, x_i \in \{0, 1\}$$

with the following transformation:

- $\forall i \in [1; n], v_i = T_i - t_i$
- $\forall i \in [1; n], w_i = S_i - s_i$
- $\mathcal{W} = \mathcal{M} - \sum_{i=1}^n s_i$

Therefore, *Knapsack* and *MakespanWithBoundedMemory* are equivalent.

The *Knapsack* problem is known to be NP-complete, however efficient approximation algorithms have been derived. The equivalence of our two problems does not a priori hold for the approximations, especially since *MakespanWithBoundedMemory* is a minimization problem where *Knapsack* is a maximization problem. We prove in the following theorem that this is indeed the case.

Theorem 2 *Any λ -approximation algorithm for Knapsack results in a λ -approximation algorithm for MakespanWithBoundedMemory.*

Proof 2 We consider a λ -approximation algorithm $\text{Algo}_{\text{approx}}$ and an optimal algorithm Opt for *Knapsack*. We consider the solution of $\text{Algo}_{\text{approx}}$ applied on the instance of the *MakespanWithBoundedMemory* problem transformed as explained above. We note:

- $t_{\text{base}} = \sum_{i=1}^n t_i \geq 0$.
- I the set of tasks chosen by $\text{Algo}_{\text{approx}}$
- J the set of tasks chosen by Opt .

Therefore, the optimal value of *Knapsack* is $\sum_{i \in J} (T_i - t_i)$.

We know from the equivalence of the previous theorem that the optimal time for *MakespanWithBoundedMemory* is $T_{\text{Opt}} = t_{\text{base}} + \sum_{i \in J} (T_i - t_i)$.

$\text{Algo}_{\text{approx}}$ is a λ -approximation for *Knapsack*. Thus, $\sum_{i \in I} (T_i - t_i) \geq \frac{1}{\lambda} \sum_{i \in J} (T_i - t_i)$. Then we know that the result delivered by $\text{Algo}_{\text{approx}}$ is:

$$\begin{aligned} T_{\text{Algo}_{\text{approx}}} &= t_{\text{base}} + \sum_{i \in I} (T_i - t_i) \\ &\geq t_{\text{base}} + \frac{1}{\lambda} \sum_{i \in J} (T_i - t_i) \\ &\geq \frac{1}{\lambda} \left(t_{\text{base}} + \sum_{i \in J} (T_i - t_i) \right) \quad \text{as } t_{\text{base}} \geq 0 \\ &\geq \frac{1}{\lambda} T_{\text{Opt}}. \end{aligned}$$

This proves that the adaptation of $\text{Algo}_{\text{approx}}$ is a λ -approximation for *MakespanWithBoundedMemory*.

Thus, we can use the Fully Polynomial-Time Approximation Scheme for *Knapsack* to solve our problem, or any other approximation scheme. In the following, we use a 2-approximation algorithm based on a refined greedy algorithm [18] described in Algorithm 1, as it provides a good solution with only $O(n \log(n))$ complexity. A lower bound on the achievable makespan can be computed using the classical greedy algorithm for the fractional *Knapsack* problem¹. This allows us to verify that the solution of Algorithm 1 is very close to optimal in all following experiments.

Algorithm 1: 2-approximation algorithm for *MakespanWithBounded-Memory*

Sort tasks by non-increasing $\frac{T_i - t_i}{S_i - s_i}$ values
 Greedily add tasks to a set S while the sum of their weights
 $w_i = S_i - s_i$ does not exceed $\mathcal{M} - \sum_{i=1}^n s_i$
 Let j be the index of the first task not selected in S
 Compare solutions S and $\{j\}$ and return the one with best makespan²

4 Predictive models to estimate time and memory

Now that we have formalized the problem and presented an approximation algorithm to compute a good solution, there is still some work to do before being able to use the proposed approach. Indeed, for each block, we need to know a priori its time and memory usage under both *early* and *lazy* modes. In Section 4.1, we list the values required to use the *memory-aware* strategy and what is available before the factorization. In Section 4.2 we present the rank model and in Section 4.3 the models used to predict the time for both strategies. In Section 4.4, we discuss the practical details of building these models, before presenting the results in Section 4.5.

4.1 Values required for the *memory-aware* strategy

In order to establish the *memory-aware* strategy, Algorithm 1 sorts values accordingly to $\frac{T_i - t_i}{S_i - s_i}$ for each block C_i of size $m_i \times n_i$. S_i corresponds to the memory required by the *lazy* mode, it is equal to the full-rank memory: $S_i = m_i \times n_i$. s_i is the memory for the *early* mode and depends on the rank of the block, denoted by r_i . Remember that we suppose that the rank of a block is constant throughout the factorization and thus equal to its final value. We also assume that the final ranks are the same for both modes. The second assumption holds

¹It consists in using Algorithm 1 to construct the set S , and adding a fraction of task j into S to completely fill the memory.

²In practice, S is always the best choice, but comparing against $\{j\}$ is required for the approximation ratio.

in practice while it would be too difficult to predict the rank evolution. Thus, we have $s_i = (m_i + n_i)r_i$. t_i is the total update time of C_i in *lazy* mode, *i.e.*, the sum of all elementary updates applied to the block C_i in *lazy* mode (cf. Figure 2(e)), while T_i is the same value for the *early* mode (cf. Figure 2(d)).

Unfortunately, we do not know the rank of blocks before the factorization. Indeed, it depends on numerical properties of the matrix and cannot be deduced only from static properties. As the cost of operations depends on the rank, we do not have access to t_i and T_i either. Thus, we have introduced models to estimate the values of s_i , t_i , and T_i .

4.2 Rank model

The first model concerns the rank, which is required to estimate both the memory storage s_i for the *early* mode and the processing times in both modes. To build this model, we rely on a linear regression. First, the simplicity of this approach makes the model easily usable in another code. Then, as the time models presented in Section 4.3 are built as linear combinations of the theoretical complexity of each operation, using a linear model for the rank simplifies the global approach.

Again remember that our objective is to estimate the final rank of a block C and not its evolution throughout the factorization. We know that this value depends on the size of the matrix but also on numerical and geometric properties. Here, we suppose that the final rank of a block depends linearly on 1) the initial rank of the block C , 2) its height m_i , 3) its width n_i , 4) the surface of the block $m_i n_i$ and 5) the number of updates the block receives. Except 1), all those data can be easily extracted from the block-symbolic factorization. As there exist methods to roughly estimate the rank of a block without fully compressing it [19], computing the initial rank is not expensive.

In order to build this model, we used as training set the previously listed parameters as well as the actual ranks for all blocks of a training matrix. Then we made a linear regression on the ranks as a linear function of the listed parameters.

4.3 Time model

In order to predict t_i and T_i , the approach consists of predicting the execution time of each elementary update, *i.e.*, *Low-rank update* and *Dense update* kernels in the DAGs on Figure 2(a). As already presented on Figure 2(d) and Figure 2(e), an update is an operation between three blocks A , B , and C that performs the operation $C = C - AB^t$.

For the full-rank case, this operation is simply a matrix-matrix product. However, in the low-rank case, both A and B can be low-rank matrices and C is either full-rank for the *lazy* mode or low-rank for the *early* mode. Thus, this update is broken down into smaller operations as presented in [3].

Depending on the strategy used, the update process can be seen as p operations op_1, \dots, op_p . Each elemental operation op_i has a theoretical complexity

which depends on the characteristics of the input matrices A , B , and C [3]. Thus, we know that T_i and t_i are a linear combination of op_1, \dots, op_p and can be obtained using a linear model. This type of approach was for instance used to obtain a better scheduling in the QR-MUMPS solver [20].

The issue is that most operations here depend on the ranks of matrices A , B , or C . A first idea would be to directly use the ranks obtained by the model presented in Section 4.2. However, one could fear that injecting the result of one model in another one would lead errors from both models to add up. Instead, we replace each occurrence of a rank (r_A , r_B , or r_C) by a linear combination of the five parameters presented in Section 4.2. This increases the number of parameters for the linear regression but avoids combining errors.

4.4 Practical details

In practice, we do not use a single model for the *early* mode. Indeed, when performing the product AB^t before updating C , there is some internal recompression process and the internal rank depends on properties of matrices A and B .

For a sparse supernodal solver like PASTIX, there are many off-diagonal blocks of different sizes. As presented in Section 2.1, large column blocks are split to exhibit more parallelism. In practice, the splitting of large column blocks is done to build column blocks with a width between 128 and 256. From the block-symbolic factorization obtained afterwards, off-diagonal blocks with a width larger or equal to 128 and a height larger or equal to 20 are marked as compressible. It means that there are a lot of small blocks that will never be compressed.

Depending on the properties of A and B , the efficiency of computing the contribution AB^t may vary. Thus, we split the original dataset into three subsets, following which blocks are marked as compressible. A first one contains updates where both A and B are compressible, a second one where exactly one matrix among A and B is compressible, and a last one where both A and B are not compressible. Then, three regressions are performed independently, one on each set to estimate the cost of elementary updates, before merging the results block by block to obtain the value of T_i .

This approach has not been proven efficient for the *lazy* mode, for which we keep a single regression.

4.5 Results of the models

In this section we present some evaluation of our models. These models predict the rank of blocks and their execution times both under the *early* and *lazy* modes. More than the predicted execution times, what matters to our approach is the ordering of blocks according to the $\frac{T_i - t_i}{S_i - s_i}$ ratio. We are therefore going to compare this ordering according to the actual values and to the predicted ones.

However, before all, we should notice that there are blocks for which one mode is the best whatever the context. Let us consider a block C_i of size

$m_i \times n_i$. If C_i uses more memory when compressed than when uncompressed ($s_i \geq S_i$), there is no memory advantage to compress it, we always run it under the *lazy* mode, and we label it LAZY. Otherwise, if C_i executes faster under the *early* mode than under the *lazy* mode ($T_i \leq t_i$), then C_i should always be executed under the *early* mode and we label it EARLY. In all other cases, the mode under which to process C_i is *To Be Determined* by the approximation algorithm and C_i is marked TBD.

We start by assessing the quality of our partitioning of blocks into EARLY, LAZY, and TBD in Table 2 using matrix **Geo1438** which includes 56727 compressible (large enough) blocks. The training was performed using matrix **Serena** and the low-rank tolerance used for both matrices is 10^{-8} . This table leads to mixed conclusions. On the one hand, the number of actual EARLY blocks predicted as LAZY, and the number of actual LAZY blocks predicted as EARLY is negligible (3 in total). On the other hand, only 45.95% of the actual LAZY blocks are predicted as such, and 29.61% of the actual EARLY blocks are predicted as such. Moreover, 8.58% of the actual TBD blocks are predicted to be either EARLY or LAZY. Overall, the results presented by Table 2 are therefore far from being random results, but they are also not perfect and the approximation algorithm will have to process significantly more blocks than required if we had a perfect oracle.

Predicted \ Actual	EARLY	TBD	LAZY	Total
	EARLY	TBD	LAZY	Total
EARLY	10.76%	3.54%	0.00%	14.30%
TBD	25.57%	49.72%	5.01%	80.30%
LAZY	0.00%	1.13%	4.26%	5.39%
Total	36.33%	54.39%	9.28%	100%

Table 2: Statistics on the classification of blocks according to their actual and predicted characteristics.

In Figure 3 we compare the ordering of all blocks when using either the actual characteristics of blocks or the predicted ones. For both sets of characteristics, EARLY blocks are ordered first, then the TBD blocks, and finally the LAZY blocks. The TBD blocks are obviously ordered according to the $\frac{T_i - t_i}{S_i - s_i}$ ratio. The other blocks are (arbitrarily) ordered using the block identifiers. This explains why the set of correctly predicted EARLY blocks forms a (light blue) line on the graph, and so do the correctly predicted LAZY blocks (dark green line). In this figure blocks are colored according to both their actual (suffix “Act”) and predicted (suffix “Pred”) types.

Once again, the conclusions are mixed. On the one hand, this figure does not look at all like a random figure (where sub-rectangles would be uniformly filled). For instance, the mislabelled actual EARLY blocks (dark blue dots) appear rather “early” in the overall order and the mislabelled actual LAZY blocks (pink dots) appear mostly very late in the order. Also, one can guess a trend looking like a diagonal for the actual TBD blocks that are correctly predicted (dark orange

dots).

On the other hand, one could argue that the clouds of points show huge variations in the ordering of some blocks. One might wonder, however, whether changing the position of a block in the ordering by 1000 (or 5000) positions in a list of more than 56000 blocks really matters. The actual question is whether such mixed results for the ordering of blocks can still lead to an efficient heuristic in practice. (As we dared to submit this paper, the reader can guess that the answer to that question is positive, at least in our minds.)

As a side note, we remark that, in practice, the quality of the solution produced by Algorithm 1 is not distinguishable from the quality of the optimal solution.

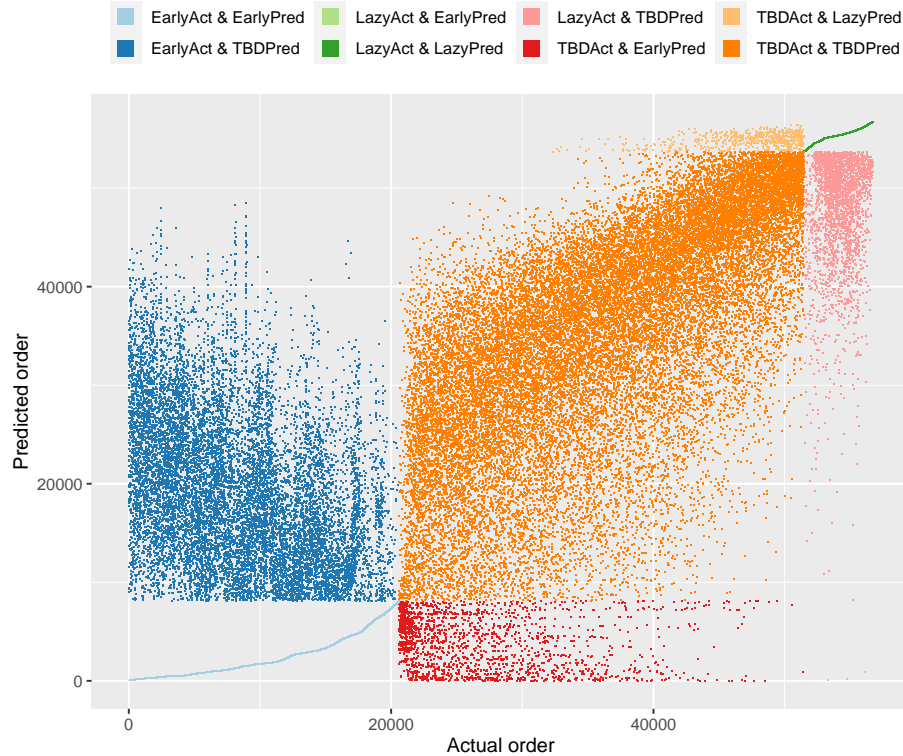


Figure 3: Comparison of the actual and predicted orders of blocks, under Algorithm 1.

5 Experiments

We now present the results of our *memory-aware* strategy. In Section 5.1, we present the machine as well as the matrices used for the experiments. In

Section 5.2, we detail the implementation of the memory-aware strategy. In Section 5.3, we demonstrate the potential of the method. In Section 5.4, we comment on the implementation of this approach into the PASTIX solver before detailing results on factorization time in Section 5.5.

5.1 Experimental context

Experiments were performed on the `crunch` cluster from our LIP laboratory, where a node is equipped with four INTEL XEON E5-4620 8-cores running at 2.20 GHz and 378 GB of memory. On this platform, the INTEL MKL 2018 library is used for sequential BLAS and LAPACK kernels. The PASTIX version used for our experiments is based on the public git repository³ version at the tag 6.1.0. Large column blocks are split in order to obtain column blocks of width between 128 and 256. Blocks with a width larger or equal to 128 and a height larger or equal to 20 are set to compressible. In all those experiments, a 10^{-8} tolerance has been used.

In order to validate the results for representative real-life problems, we have used five 3D matrices extracted from The SuiteSparse Matrix Collection [21]:

- **Atmosmod1**: atmospheric model (1 489 752 non-zeroes)
- **Flan1565**: 3D mechanical problem discretizing a steel flange (1 564 794 non-zeroes)
- **Geo1438**: geomechanical model of earth (1 437 960 non-zeroes)
- **Hook1498**: model of a steel hook (1 498 023 non-zeroes)
- **Serena**: gas reservoir simulation (1 391 349 non-zeroes)

Note that these matrices come from different application fields and have thus different mathematical properties. Therefore, training the model on a matrix and using it for another matrix will test not only the efficiency of the model, but also the robustness of our overall approach. Our objective here is to predict memory consumption and computational cost using the models presented in Section 4.2 and Section 4.3, and to use these values to select which blocks to execute in *lazy* mode in order to use as much memory as possible without overcoming a given memory limit.

5.2 Implementation of the *memory-aware* strategy

In this section, we present how we solve the *MakespanWithBoundedMemory* problem presented in Section 3 in practice. The choice of the mode for blocks (*early* or *lazy*) is done in a dynamic way before their allocation in the memory. We describe in detail the approach below.

³<https://gitlab.inria.fr/solverstack/pastix>

1. For both training and test matrices, we run the real factorization using *Just-In-Time* and *Minimal Memory* strategies for all blocks. Then we extract information for each elementary update, using results of the *Minimal Memory* (respectively *Just-In-Time*) for the *early* (resp. *lazy*) mode. We perform three runs and take the median value to remove data noise before training the model. Then, we compute the rank model and both time models;
2. We select blocks that should always be treated in *lazy* mode ($s_i \geq S_i$) as well as blocks that should always be treated in *early* mode ($t_i \geq T_i$);
3. We sort the remaining blocks with the greedy algorithm presented in Algorithm 1 by decreasing value of $\frac{T_i - t_i}{S_i - s_i}$;
4. We consider all remaining blocks in *lazy* mode (uncompressed), which would all require S_i if allocated in memory. Then, some blocks are compressed (and thus moved to the *early* mode) following the previous order until the memory limit is achieved. The memory consumption of the current solution is computed as the sum of S_i for blocks still in the *lazy* mode plus the sum of the s_i for blocks moved to *early* mode. Note that we use the real size s_i and not the predicted one: it is known as soon as a block is compressed (and it is more accurate than the predicted one). When the memory of the current solution falls below the memory limit, blocks still in *lazy* mode may safely be loaded.

5.3 Potential gain estimation through simulation

In order to validate the models presented in Section 4, we have implemented the previous approach using different ordering strategies for Step 3. From now on, we denote by T_i , t_i , and s_i the actual timings and memory consumption and T_i^* , t_i^* , and s_i^* the predicted ones. The four orderings are:

- Decreasing **theoretical ratio** $\frac{T_i - t_i}{S_i - s_i}$ (this is to get a bound on the best result we can obtain with our models).
- Decreasing **predicted ratio** $\frac{T_i^* - t_i^*}{S_i - s_i^*}$ (original strategy).
- Decreasing number of updates received by a block: we expect blocks receiving many updates to be more efficient in *lazy* mode, to avoid numerous expensive low-rank updates (denoted by **count** in the following figures). This strategies does not rely on predicted values, and is thus simpler to implement.
- **Random** order, for baseline comparison.

On Figure 4, we present the results of the four heuristics for the **Geo1438** matrix. The training of the models was realized with the **Serena** matrix. Both matrices were studied with a 10^{-8} tolerance. For each possible memory limit,

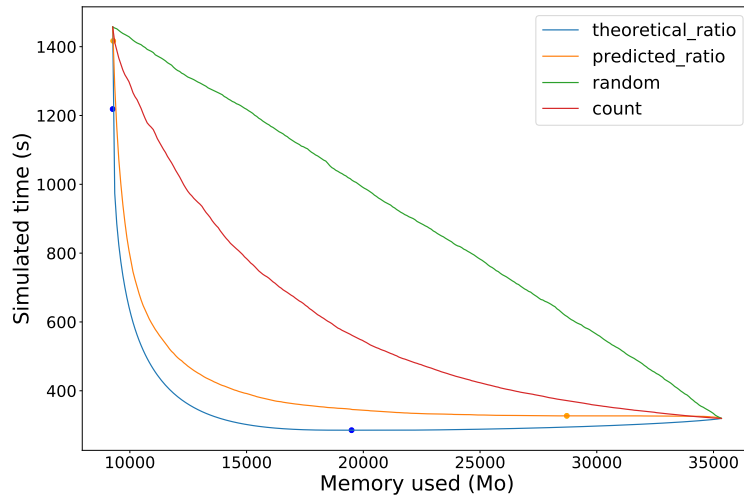


Figure 4: Simulated time of update tasks depending on the memory constraint for Geo1438 solved with a 10^{-8} tolerance for four different heuristics. The training matrix for the predictive strategy is Serena using a 10^{-8} tolerance. The top-left point represents the *Minimal Memory* strategy while the bottom-right point represents the *Just-In-Time* strategy.

we run the previous algorithm to decide which mode to use for each block. Note that here, the time is simulated and corresponds only to the sum of update times; the cost of common operations (remaining kernels of the considered blocks as well as all operations on small full-rank blocks such as the factorization of diagonal blocks) is omitted for better readability. The update times are extracted from the training data set, as explained above. On top-left part of the figure, we have the largest execution time and the lowest memory consumption: it corresponds to performing all blocks under the *early* mode, which is exactly the *Minimal Memory* strategy. On bottom-right, we have the opposite case, using *lazy* mode for all blocks, which is exactly the *Just-In-Time* strategy, with the largest memory consumption but the lowest execution time. Four points appear on the figure, two for the “theoretical ratio” and two for “predicted ratio”. The points on the left represent the lowest execution time achievable under the condition of using as low memory as possible: all blocks are executed in *early* mode except those which do not bring memory savings ($s_i \geq S_i$ or $s_i^* \geq S_i^*$) that are processed in *lazy* mode. On the contrary, the two right points represent the lowest memory consumption under the condition of being as fast as possible: all blocks are executed in *lazy* mode except those which are faster in *early* mode ($t_i \geq T_i$ or $t_i^* \geq T_i^*$).

Between those two points, one can observe all possible combinations for the *memory-aware* strategy. The first observation is that, while being not as good as the best ratio available, the prediction leads to much better results than a naive sorting such as the number of updates. In addition, one can see that interesting trade-offs between time and memory can be achieved: for instance by increasing memory consumption by only 20%, execution time can be divided by 3.

On Figure 5, one can observe the behavior of the best ratio and the predictive one for the 25 combinations. Among the five matrices we used for our experiments, we vary both the training and the testing sets, always using a 10^{-8} tolerance. This demonstrates that the results using the predictive models are often or always close to the optimal solution. This prove that our approach is very robust to the choice of the training matrix. They are similar to Figure 4 and show the robustness of our approach.

5.4 Integration of the *memory-aware* strategy into the PaStiX solver

Based on these attractive preliminary results, we now present how this *memory-aware* strategy has been introduced into the PASTIX solver and the gains obtained on actual factorization time and memory usage.

The first step consists of selecting blocks which will be performed in the *early* mode, such that the memory consumption of the factors before the factorization starts is below the given memory limit. Then, we have two opposite behaviors during the factorization. On one hand, once blocks which are managed in *lazy* mode have received all their contributions (cf. Figure 2(e)), they can be compressed, reducing the memory footprint of the solver. On the other

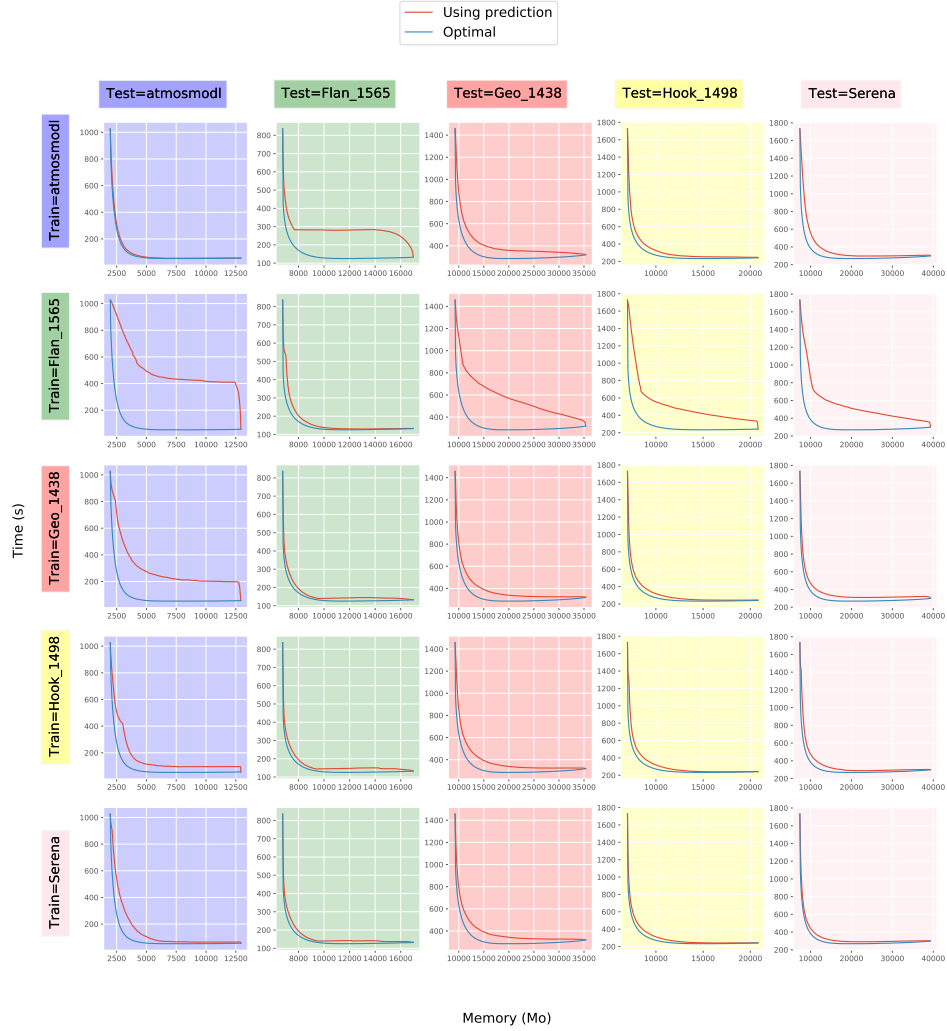


Figure 5: Execution time of update tasks depending on the memory constraint for five matrices using a 10^{-8} tolerance. For each line, the same training matrix is used and for each column the same test matrix is used. Two curves are plotted, the best results achievable knowing all information and the results obtained by our predictive models.

hand, low-rank blocks managed under *early* mode can see their rank increase due to updates (cf. Figure 2(d)), increasing the memory footprint. Thus, to ensure that we always stay under the memory limit, each time a low-rank block size increases, some extra blocks may be moved dynamically to *early* mode and compressed if the extra memory allocated would exceed the given limit.

This implementation is a proof-of-concept and has some limitations. Firstly, it is only sequential for now, as compressing on-the-fly data blocks may induce deadlocks when using PaStiX in parallel. Secondly, building and using the models as well as sorting blocks is performed using an external tool. In future work, it will be fully integrated into the PaStiX solver, and a parallel memory management will be proposed.

5.5 Real gain for the PaStiX solver

With the implementation presented before, we can now compare the behavior of both *Just-In-Time* and *Minimal Memory* strategies with the *memory-aware* method introduced in this paper. This requires to add an extra entry parameter to the PaStiX solver, the maximum memory authorized.

In Table 3 we present, for five matrices solved at tolerance 10^{-8} , the memory consumption and factorization time for the *Just-In-Time* and *Minimal Memory* strategies. The models were trained using the *Serena* matrix with a 10^{-8} tolerance. We evaluate the *memory-aware* strategy with different memory limits, as well as two extreme cases: all blocks executed in *early* mode except those which do not bring memory savings (denoted *minimum*) and all blocks executed in *lazy* mode except those which do not reduce execution time (denoted ∞). We present both the optimal time (using actual values from the execution) and the time achieved using the predictive models. The results demonstrate that an interesting trade-off between time and memory can always be achieved. For instance, for the *Geo1438* matrix, increasing memory consumption by 30% divides by 2.2 the execution time of *Minimal Memory* strategy. Similarly, 60% of the memory consumption of the *Just-In-Time* strategy could be saved by increasing by only 10% the execution time. Using the predictive values we are always within 10% of the optimal performance.

6 Conclusion

In sparse direct solvers, using low-rank compression has emerged as a solution to process larger matrices. Existing solvers use either only low-rank updates (the matrix is compressed beforehand) or only full-rank updates (the matrix is compressed during the factorization). We have presented a *memory-aware* approach, performing both types of updates, whose objective is to enable applications to run as fast as possible while keeping their memory usage under a given memory limit (e.g., the size of the RAM).

We have formalized the optimization problem of choosing which blocks to compress in the *early* or *lazy* mode, and shown its equivalence to the knapsack

problem, which proves our problem NP-complete. We have successfully adapted a 2-approximation algorithm for our problem.

To take advantage of this optimization algorithm, we need information on matrix blocks (memory consumption once compressed, processing time in both modes) which is usually unknown before the computation. To leverage this problem, we have introduced models to predict these values. We have demonstrated that using these models we can achieve a performance close to the results achievable with a perfect omniscient oracle, even in the less favorable case where the models are trained with a matrix from one application field and used with matrices from another field. Our approach sorts all blocks and selects at runtime, depending on the actual memory usage, which ones to manage with low-rank updates (*early* mode) and which ones to manage with full-rank updates (*lazy* mode). This ensures that the memory bound is respected.

Our *memory-aware* strategy has been integrated into the PASTIX solver. The obtained execution times are far lower than the existing memory-conservative strategy (for instance, twice faster), even for memory limits that are only slightly larger than the memory usage of this strategy (for instance, 30% increase in memory). Conversely, it is only marginally slower than the performance-oriented strategy (for instance, 10% increase in execution time) while using drastically less memory (for instance, half the memory). The *memory-aware* strategy thus achieves a kind of “best of both world” performance, allowing a wide range of memory-time trade-offs.

The implementation is for now sequential and the memory management has to be adapted for the parallel case, which is left for future work. The main problem here is to avoid deadlocks, as the next candidate for being compressed may be used by another thread, for instance to apply an update. The work conducted in [22] could be a starting point.

Another future work consists of using geometric information of the matrix, which is known to influence ranks, to try to enhance the predictive models of processing times and memory consumption.

Up to our knowledge, this work is the first tentative to produce models for low-rank compression in the sparse case. It could be used to exhibit better time estimation to enhance scheduling for sparse direct solvers using low-rank compression.

Acknowledgments

This work is part of the SOLHARIS project, supported by the Agence Nationale de la Recherche, under grant ANR-19-CE46-0009.

References

- [1] P. R. Amestoy, C. Ashcraft, O. Boiteau, A. Buttari, J.-Y. L’Excellent, and C. Weisbecker, “Improving Multifrontal Methods by Means of Block Low-

- Rank Representations,” *SIAM Journal on Scientific Computing*, vol. 37, no. 3, pp. A1451–A1474, 2015.
- [2] T. Mary, “Block Low-Rank multifrontal solvers: complexity, performance, and scalability,” Ph.D. dissertation, Toulouse University, Toulouse, France, Nov. 2017.
 - [3] G. Pichon, “On the use of low-rank arithmetic to reduce the complexity of parallel sparse linear solvers based on direct factorization techniques,” Ph.D. dissertation, Université de Bordeaux, Talence, France, Nov. 2018.
 - [4] W. Hackbusch, “A Sparse Matrix Arithmetic Based on \mathcal{H} -Matrices. Part I: Introduction to \mathcal{H} -Matrices,” *Computing*, vol. 62, no. 2, pp. 89–108, 1999.
 - [5] W. Hackbusch and S. Börm, “Data-sparse Approximation by Adaptive \mathcal{H}^2 -Matrices,” *Computing*, vol. 69, no. 1, pp. 1–35, 2002.
 - [6] P. Ghysels, X. S. Li, C. Gorman, and F.-H. Rouet, “A robust parallel preconditioner for indefinite systems using hierarchical matrices and randomized sampling,” in *2017 IEEE IPDPS*, 2017, pp. 897–906.
 - [7] A. Aminfar and E. Darve, “A fast, memory efficient and robust sparse preconditioner based on a multifrontal approach with applications to finite-element matrices,” *International Journal for Numerical Methods in Engineering*, vol. 107, no. 6, pp. 520–540, 2016.
 - [8] T. A. Davis, R. Sivasankaran, and W. M. Sid-Lakhdar, “A survey of direct methods for sparse linear systems,” *Acta Numerica*, vol. 25, pp. 383–566, 2016.
 - [9] A. George, “Nested dissection of a regular finite element mesh,” *SIAM Journal on Numerical Analysis*, vol. 10, no. 2, pp. 345–363, 1973.
 - [10] G. Karypis and V. Kumar, “METIS: A software package for partitioning unstructured graphs, partitioning meshes, and computing fill-reducing orderings of sparse matrices,” 1995.
 - [11] F. Pellegrini, “Scotch and libScotch 5.1 User’s Guide,” Aug. 2008, user’s manual, 127 pages.
 - [12] J. J. Dongarra, J. Du Croz, S. Hammarling, and I. S. Duff, “A set of level 3 basic linear algebra subprograms,” *ACM Trans. Math. Softw.*, vol. 16, no. 1, pp. 1–17, 1990.
 - [13] P. Hénon, P. Ramet, and J. Roman, “PaStiX: A High-Performance Parallel Direct Solver for Sparse Symmetric Definite Systems,” *Parallel Computing*, vol. 28, no. 2, pp. 301–321, Jan. 2002.
 - [14] J. N. Chadwick and D. S. Bindel, “An Efficient Solver for Sparse Linear Systems Based on Rank-Structured Cholesky Factorization,” *CoRR*, vol. abs/1507.05593, 2015.

- [15] J. E. Savage, *Models of computation - exploring the power of computing*. Addison-Wesley, 1998.
- [16] L. Marchal, “Memory and data aware scheduling,” Habilitation Thesis, École Normale Supérieure de Lyon, 2018.
- [17] H. Kellerer, U. Pferschy, and D. Pisinger, “Multidimensional knapsack problems,” in *Knapsack problems*. Springer, 2004, pp. 235–283.
- [18] E. Tardos, “Introduction to approximation and online algorithms,” available online at <http://www.cs.cornell.edu/courses/cs4820/2018fa/lectures/approx-onlinet.pdf>, course note of CS 4820 Spring 2016 “Introduction to Algorithms” at Cornell University.
- [19] S. Ubaru and Y. Saad, “Fast methods for estimating the numerical rank of large matrices,” in *ICML*, 2016, pp. 468–477.
- [20] L. Stanislav, E. Agullo, A. Buttari, A. Guermouche, A. Legrand, F. Lopez, and B. Videau, “Fast and accurate simulation of multithreaded sparse linear algebra solvers,” *2015 IEEE ICPADS*, 2015.
- [21] T. A. Davis and Y. Hu, “The University of Florida sparse matrix collection,” *ACM Trans. Math. Softw.*, vol. 38, no. 1, Dec. 2011.
- [22] M. Sergent, D. Goudin, S. Thibault, and O. Aumage, “Controlling the Memory Subscription of Distributed Applications with a Task-Based Runtime System,” in *HIPS*, Chicago, IL, May 2016.

Table 3: Factorization time and memory consumption for five matrices solved at tolerance 10^{-8} . For each matrix, the results of both *Just-In-Time* (JIT) and *Minimal Memory* (MM) are presented as well as the results for different *memory-aware* strategies where the memory limit varies. For the *memory-aware* strategy, the predictive model is obtained using Serena as training test. Two information are provided, the best result achievable knowing all information and the result obtained using our predictive model.

Matrix	Strategy	Memory (GB)	Time(s)	
			With pred (s)	Opt time (s)
atmosmodl	<i>Just-In-Time</i>	16.9		142.5
	<i>Minimal Memory</i>	5.64		1112.5
		minimum	750.6	795.3
		6	535.4	397.4
	<i>memory-aware</i>	9	176.7	143.0
		12	148.3	138.4
		∞	148.5	140.7
Flan1565	<i>Just-In-Time</i>	26.4		273.1
	<i>Minimal Memory</i>	13.9		922.5
		minimum	490.5	456.2
		14	433.3	431.2
	<i>memory-aware</i>	16	332.7	347.2
		18	288.9	281.8
		∞	286.2	268.9
Geo1438	<i>Just-In-Time</i>	43.2		555.9
	<i>Minimal Memory</i>	14.7		1591.7
		minimum	1190.2	1149.1
		19	724.1	647.0
	<i>memory-aware</i>	23	663.3	576.0
		27	618.6	556.5
		∞	578.3	553.9
Hook1498	<i>Just-In-Time</i>	27.2		407.3
	<i>Minimal Memory</i>	11.8		1863.7
		minimum	1056.1	991.5
		16	506.4	465.3
	<i>memory-aware</i>	20	431.9	417.0
		24	416.5	410.0
		∞	415.5	412.3
Serena	<i>Just-In-Time</i>	46.7		534.2
	<i>Minimal Memory</i>	13.3		1876.2
		minimum	1300.5	1270.9
		18	654.0	606.0
	<i>memory-aware</i>	22	579.1	543.5
		26	552.7	529.1
		∞	539.8	527.1



**RESEARCH CENTRE
GRENOBLE – RHÔNE-ALPES**

Inovallée
655 avenue de l'Europe Montbonnot
38334 Saint Ismier Cedex

Publisher
Inria
Domaine de Voluceau - Rocquencourt
BP 105 - 78153 Le Chesnay Cedex
inria.fr

ISSN 0249-6399